

ABSTRACT

A method of easily and speedily determining what structural change is experienced by a target protein upon contact and binding of any arbitrary compound to the target protein; a method of selecting and screening a compound for use in the method; and a computer program for carrying out these methods. In one embodiment, a Saupe order matrix element of domain is obtained from atomic coordinates of domain and an axial-direction variation of NMR signal dependent upon the orientation angle of molecule in magnetic field, and the matrix is diagonalized to thereby obtain the orientation information on the domain. Using of any change of the orientation information as an indicator for structural change enables realization of the intended easy and speedy measurement of structural change of the target protein.